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Title: **PRESENT STATE OF THE SOURCES COMPUTER CODE**

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PRESENT STATE OF THE SOURCES COMPUTER CODE

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SUMMARY
In various stages of development for over two decades, the SOURCES computer code continues to calculate neutron production rates and spectra from four types of problems: homogeneous media, two-region interfaces, three-region interfaces and that of a monoenergetic alpha particle beam incident on a slab of target material.[1]

Graduate work at the University of Missouri – Rolla, in addition to user feedback from a tutorial course, provided the impetus for a variety of code improvements. Recently upgraded to version 4B, initial modifications to SOURCES focused on updates to the "tape5" decay data library. Shortly thereafter, efforts focused on development of a graphical user interface for the code. This paper documents the Los Alamos SOURCES Tape1 Creator and Library Link (LASTCALL) and describes additional library modifications in more detail. Minor improvements and planned enhancements are discussed.

I. HISTORY
The following section was written for the updated user's manual planned for release during the next major code upgrade (version 5A).

The SOURCES-5A code has been under development since the early 1980's with continuing improvements made in both methods and data. Effectively version 1.0, the original version of SOURCES was actually named POFEAL and primarily used for calculating the probability of an (α,n) interaction with nuclide i by an alpha particle prior to stopping in the material (P_i OF E-ALpha).[2] Developed by the Los Alamos Applied Nuclear Science Group (then T-2), the code was intended to calculate neutron production in source materials such as oxide and carbide fuels, plutonium metal, aqueous process solutions, and uranium enrichment processes. The Safeguards Technology Group (then Q-1) furthered interest and POFEAL's capabilities were improved by including spectral calculations and making adjustments to the calculational algorithms.[3] It was during this time in 1982 when the code was actually referred to as SOURCES and distinguished from POFEAL. Although often assumed an acronym, SOURCES was simply a name for the code given by the primary developer, W.B. Wilson. In addition to the original probability calculations, SOURCES (effectively version 2.0) was then able to calculate neutron "sources" from the spontaneous fission of actinide nuclides, the (α,n) reactions of their decay alpha particles with light nuclides, and delayed neutrons.

Public release via the Radiation Safety Information Computational Center (RSICC) required both a "frozen" version of the code for control purposes and a method to track changes. Consequently, a naming convention was chosen in 1997 when the two-region interface problem was added. In place for version 3A, the new convention designated a trailing numeral to indicate a major code release followed by a letter to designate any minor improvements. Thus version 3A was the third major version of the code. The capability to calculate (α,n) source rates and spectra for three-region interface problems was added for 1999's version 4A. Minor data improvements to the tape5 library upgraded version 4A to 4B in 2001. Although a user's manual did not exist until version 3A, and versions 4A and 5A each were issued with an updated manual, minor upgrades typically would not warrant efforts to produce a revised document. The user is encouraged to monitor the code distributor's (RSICC) publications (e.g. newsletter and web-site) for updates, notices, and associated documentation related to any improvements.

Existing for both unix and DOS-based computing platforms, SOURCES-5A currently consists of a FORTRAN 77 (F77) source code, a user-created input file, up to six output files, and four library files. The user's manual is applicable for both types of computing platforms although installation may vary on each system. Appendix C of the

manual includes many works related to SOURCES not expressly referenced in the documentation. These references may provide the reader with additional information regarding the historical development and theory behind the SOURCES code.

The code and manual are not static. They will continue to be improved and updated as more experimental data and computational methods become available, new features are desired, and as time permits. The code continues to be available from RSICC, a computer code center authorized to collect, maintain, and distribute computer software in the areas of radiation transport and safety.

The success of SOURCES is dependent upon input from the user community. Rigorous manipulations of the code under a variety of conditions expose weaknesses that might otherwise go undetected. Any error reports or suggestions for improvement are certainly welcomed. Furthermore, additional benchmarking problems and data sources are continually being sought for validation purposes. Such contributions should be sent to the current code custodian at Los Alamos, Erik F. Shores (eshores@lanl.gov).

II. DATA UPDATES

Because alpha decay contributes to neutron spectra through (α,n) reactions, the energy and emission probability for each alpha level are important parameters. The SOURCES 4B upgrade was the result of updates to the code's decay data library (tape5) for 44 of the 105 available decay sources. The new version provided spontaneous fission information for ^{252}Cf and alpha decay data revisions for 43 isotopes and isomers having Watt fission spectra parameters.[4] Following that work, similar modifications to the remaining 63 sources were made in an effort to provide consistent, easily referenced data. Summarized elsewhere[5] the alterations reflect information found in the most recent edition of the Table of Isotopes.[6]

Among the revisions, a variety of alpha lines were added or deleted to the sources ranging from ^{142}Ce to ^{257}Fm (Table 1). Non-zero branching fractions were changed to zero for the following 14 isotopes: ^{232}U, ^{237}U, ^{239}U, ^{236}Np, ^{236m}Np, ^{238}Np, ^{239}Np, ^{237}Pu, ^{243}Pu, ^{240}Am, ^{242}Am, ^{244}Am, ^{244m}Am and ^{241}Cm. Several caveats apply regarding the various alpha decay lines specified for these nuclides. First of all, alpha energies not accompanied by an emission probability or assigned a "?" (signifying questionable existence) were omitted from tape5. In addition, any limits in the data (e.g. "<" or ">") assumed the given value for tape5 inclusion. For example, "< 1.234e-05" became "= 1.234e-05".

III. MINOR IMPROVEMENTS

When calculating neutron spectra (id = 2), a histogram of descending energy structure has been the de facto output from SOURCES. Many users, however, desired an ascending energy structure—especially those coupling SOURCES output to a transport code such as MCNP[a]. Consequently, a new option takes the form of a third record (erg) on the second card (following idd and id) to obtain an energy structure in ascending or descending order. For an ascending structure, erg=1 and for a descending structure, erg=-1. The selection of either option produces an additional output file (outp2) containing spectral histograms in a format conducive to further manipulation.

IV. THREE BODY REACTION

Discrepancies among published neutron spectra exist in lower energy (e.g. < 2 MeV) regions of problems involving beryllium as the target material. Early work (circa 1938) on beryllium (α,n) sources found evidence for the existence of neutrons with energies below 1 MeV unlikely to have originated through the population of ^{12}C levels.[7] Indeed, several authors suggested a three-body breakup reaction [e.g. ^{9}Be (α,α') ^{9}Be* = ^{8}Be + n] as the production mechanism. This reaction path, yielding "low-energy neutrons over a wide range of alpha particle energies," results from inelastic scattering of alpha particles.[8] Although some recent works (e.g. Faw and Shultis[9]) also mention these "lower energy neutrons," many other references summarizing (α,n) sources do not mention this path. Not currently considered by SOURCES in terms of spectral calculations (although the neutron production magnitudes are accounted for via beryllium's well known total cross section), analysis of spectral affects from the addition of this mechanism continues to be a pursued via graduate work at the University of Missouri-Rolla.

[a] MCNP is a trademark of the Regents of the University of California, Los Alamos National Laboratory

Table 1. Actinide Isotopes Available as Decay Sources in SOURCES 5A.

	Isotope	ZAID
1	Ce-142	581420
2	Nd-144	601440
3	Sm-146	621460
4	Sm-147	621470
5	Sm-148	621480
6	Sm-149	621490
7	Gd-152	641520
8	Pb-210	822100
9	Bi-210	832100
10	Bi-211	832110
11	Bi-212	832120
12	Bi-213	832130
13	Bi-214	832140
14	Po-210	842100
15	Po-211	842110
16	Po-212	842120
17	Po-213	842130
18	Po-214	842140
19	Po-215	842150
20	Po-216	842160
21	Po-218	842180
22	At-215	852150
23	At-217	852170
24	At-218	852180
25	At-219	852190
26	Rn-217	862170
27	Rn-218	862180
28	Rn-219	862190
29	Rn-220	862200
30	Rn-222	862220
31	Fr-221	872210
32	Fr-222	872220
33	Fr-223	872230
34	Ra-222	882220
35	Ra-223	882230
36	Ra-224	882240

	Isotope	ZAID
37	Ra-226	882260
38	Ac-225	892250
39	Ac-226	892260
40	Ac-227	892270
41	Th-226	902260
42	Th-227	902270
43	Th-228	902280
44	Th-229	902290
45	Th-230[sf w]	902300
46	Th-232[sf w]	902320
47	Pa-230	912300
48	Pa-231[sf w]	912310
49	U-230	922300
50	U-231	922310
51	U-232	922320
52	U-233[sf w]	922330
53	U-234[sf w]	922340
54	U-235[sf w]	922350
55	U-236[sf w]	922360
56	U-237[0]	922370
57	U-238[sf w]	922380
58	U-239[0]	922390
59	Np-235	932350
60	Np-236[0]	932360
61	Np-236m[0]	932361
62	Np-237[sf w]	932370
63	Np-238[0]	932380
64	Np-239[0]	932390
65	Pu-235	942350
66	Pu-236[sf w]	942360
67	Pu-237	942370
68	Pu-238[sf w]	942380
69	Pu-239[sf w]	942390
70	Pu-240[sf w]	942400
71	Pu-241[sf w]	942410
72	Pu-242[sf w]	942420

	Isotope	ZAID
73	Pu-243[0]	942430
74	Pu-244[sf w]	942440
75	Am-240	952400
76	Am-241[sf w]	952410
77	Am-242[0]	952420
78	Am-242m[sf w]	952421
79	Am-243[sf w]	952430
80	Am-244[0]	952440
81	Am-244m[0]	952441
82	Cm-240[sf w]	962400
83	Cm-241	962410
84	Cm-242[sf w]	962420
85	Cm-243[sf w]	962430
86	Cm-244[sf w]	962440
87	Cm-245[sf w]	962450
88	Cm-246[sf w]	962460
89	Cm-247	962470
90	Cm-248[sf w]	962480
91	Cm-250[sf w 0]	962500
92	Bk-249[sf w]	972490
93	Cf-248[sf w]	982480
94	Cf-249[sf]	982490
95	Cf-250[sf]	982500
96	Cf-251	982510
97	Cf-252[sf w]	982520
98	Cf-253	982530
99	Cf-254[sf]	982540
100	Es-253[sf]	992530
101	Es-254[sf]	992540
102	Es-254m[sf]	992541
103	Es-255[sf]	992550
104	Fm-254[sf]	1002540
105	Fm-255[sf]	1002550
106	Fm-256[sf]	1002560
107	Fm-257[sf]	1002570

[0] Denotes 11 nuclides having zero alpha emission per Firestone and Shirley.
[sf] Denotes 41 nuclides with nonzero spontaneous fission (SF) branching fractions.
[w] Denotes 30 nuclides with nonzero SF branching fractions and parameters for Watt Fission Spectra.
Note: there are 14 nuclides with Watt Fission Spectra parameters but zero SF branching fractions.

Similar to the kinematics associated with calculated minimum and maximum neutron energies produced by a given alpha for a typical two-body problem (part of the basis for SOURCES spectral output), those of a three-body problem may also be derived. Indeed, these neutron energy limits have been calculated using the derivation of Morinigo.[10] Methodology to incorporate these limits is being explored.

V. LASTCALL

In an effort to streamline the process of creating the tape1 file, the Los Alamos SOURCES Tape1 Creator and Library Link (LASTCALL) program was developed and recently introduced. Intended to supplement the SOURCES manual and make calculations simpler, LASTCALL was designed to minimize common errors and guide the novice or typical user. An optional application, LASTCALL will be on the distribution CD with the next release of SOURCES from RSICC. Any users desiring the code prior to the release should contact the author.

Written in Fortran using Compaq Visual Fortran,[11] LASTCALL consists of a simple dialog window launched from an executable. The default view is shown in Figure 1. The executable (lastcall.exe), when placed in the SOURCES directory containing that code's executable and library files, will produce an input file allowing SOURCES to run (within LASTCALL, if desired) and produce typical output files.

Like the sample problems in the SOURCES-4A manual, LASTCALL is available as an instructive device for the user. Sample problem number one [Ref 1] demonstrates a homogenous mixture problem consisting of plutonium and beryllium and was designed to model an experimental measurement by Stewart.[12] This sample problem is now used to demonstrate the use of LASTCALL.

Referring again to Figure 1, we note the window is roughly divided into seven sections. The first section, "Problem Type" is self-explanatory and defaults to a homogenous problem (Sample Problem 1). Presently, the capabilities for interface and three-region problems are unavailable and will be added as time permits. The second section, "Problem Title" is also self-explanatory. This field, limited to 77 characters, is the only comment allowed on the tape1 file. In this case, we've noted our problem is a "PuBe Neutron Source…" In the third section, a selection must be made regarding "Neutron Production Output". Options are available through a pull-down menu (Figure 2) for calculating neutron magnitudes only, or as a supplement to neutron spectra. The latter has two selections such that spectral energy bins may be presented in either ascending or descending order. The "About" button represents the optional fourth section and simply presents the name and version of the code in addition to making a solicitation for comments and suggestions regarding SOURCES or LASTCALL.

Once this preliminary information has been considered, the remaining options may be examined. The fifth section of the dialog box is a tab control subdivided into seven areas allowing description of the main portion of tape1.

After viewing some introductory material on the first tab (Figure 1), the elemental constituents for the problem may be selected on the second "Elements" tab (Figure 2). One or multiple elements may be selected from the list box "Elements by Z" and moved into "This Problem" (or vice versa) using the arrow(s). The "Elemental constituents" box summarizes the number of elements selected. The atom fraction for each element is required and may be entered via the box labeled "Element j's atom fraction". Clicking the "Enter" button transfers the entry into the "Fraction" box. Presently, this primitive entry mechanism has no method for correction. In other words, any mistakes may *not* be corrected until the tape1 file is viewed. At that point, manual corrections may be made. The fractions must be entered in the order of the elements listed in the problem box. Any entries made surpassing the number of elements will be ignored. This tab also provides the option to select solid or gas stopping cross sections. For the sample problem, we've selected two elements (beryllium and plutonium), entered their appropriate atom fractions (0.928571 and 0.071429, respectively), and chosen solid cross sections.

The third tab, "Sources", allows selection of alpha emitters existing in the problem (Figure 3). In this case, an atom density, rather than atom fraction, must be entered for each alpha source. Practically speaking, these fields are identical to those on the element tab. Had this problem been a "beam" type in lieu of a "homogeneous mixture", the "Beam Energy" field would be required. In that case, the other source fields would become disabled. For the sample problem, six plutonium isotopes were selected and appropriate atom densities entered.

At this point (Figure 3), we've elected to change the neutron production output to that revealing an energy spectrum in ascending energy bins. This selection made the sixth region of the dialog window ("Neutron Group Structure") active. The default number of groups was subsequently increased from 10 to 48. The "linearly interpolated" default between a newly modified energy range of 0.0-12.0 MeV was accepted. A pull-down menu reveals a user-defined energy structure option that allows entry of bin limits in the provided area. Such a user-defined description may not appear convenient on the generated tape1 (it is written on one continuous line) and may be manually reformatted into multiple lines, if desired.

The "Target" tab functions are analogous to the preceding two tabs. Multiple targets may be selected and appropriate atom fractions entered. This tab also allows deviation from the default number of alpha energy groups (4000). A singular target (beryllium) was selected for the sample problem. Incidentally, the atom fraction (0.928571) is derived under the assumption this plutonium-beryllium neutron source took the form of an intermetallic alloy (e.g. $PuBe_{13}$). The fraction of beryllium, therefore, is 13/14.

Three additional tabs ("Interface", "Three-Region", and "More Info") provide supplementary comments (Figure 5).

After describing the problem, the user may then consider the seventh section, "Generate Tape1, Execute, or Exit?" This section consists of three buttons. Building the tape1 files automatically opens the Microsoft® Notepad application to display the tape1 file (Figure 6). The user may continue to manually edit tape1, as necessary, and may save the file under a name other than tape1 for later manipulation or file organization purposes. Indeed, the primitive nature of this first generation interface may force additional editing, as a mechanism to correct for mis-entry does not currently exit. Figure 6 is nearly identical to the Sample Problem 1 input deck (Figure 8 of Ref 1.) and represents successful execution of LASTCALL.

Although creating the input file satisfies LASTCALL's intent, the user may now choose to execute SOURCES from the window, or exit the program. Upon successful execution, the generated output files automatically appear in the Microsoft® Notepad application; tape6 and outp in the case of a "magnitude only" calculation, and outp, outp2, and tapes6-9 in a "magnitude and spectra" calculation. Figure 7 displays a portion of the outp2 file.

To close the application, the user simply clicks the "Exit LASTCALL" button.

VI. CONCLUSIONS

The SOURCES computer code is not a static entity. Indeed, as previously noted, improvements to the code continue to be made.

The present version is 4B and a major upgrade to 5A is planned for implementation of new features such as the [^{9}Be (α,α') ^{9}Be* = ^{8}Be + n] reaction. Other improvements, such an updated user's manual, will accompany the next release.

A graphical user interface, LASTCALL, has been developed to assist users in creating tape1 input files. The use of LASTCALL was demonstrated through a SOURCES sample problem and comments regarding this Windows based application were welcomed.

ACKNOWLEDGMENTS

Thanks are due to Drs. G.E. Mueller and A. Kumar for supporting graduate work at the University of Missouri-Rolla. From LANL, Drs. W.B. Wilson, R.T. Perry, and K.D. Veal deserve thanks for discussions and a variety of useful suggestions during the course of this work. J.A. Sattelberger's assistance with updating the data files was appreciated.

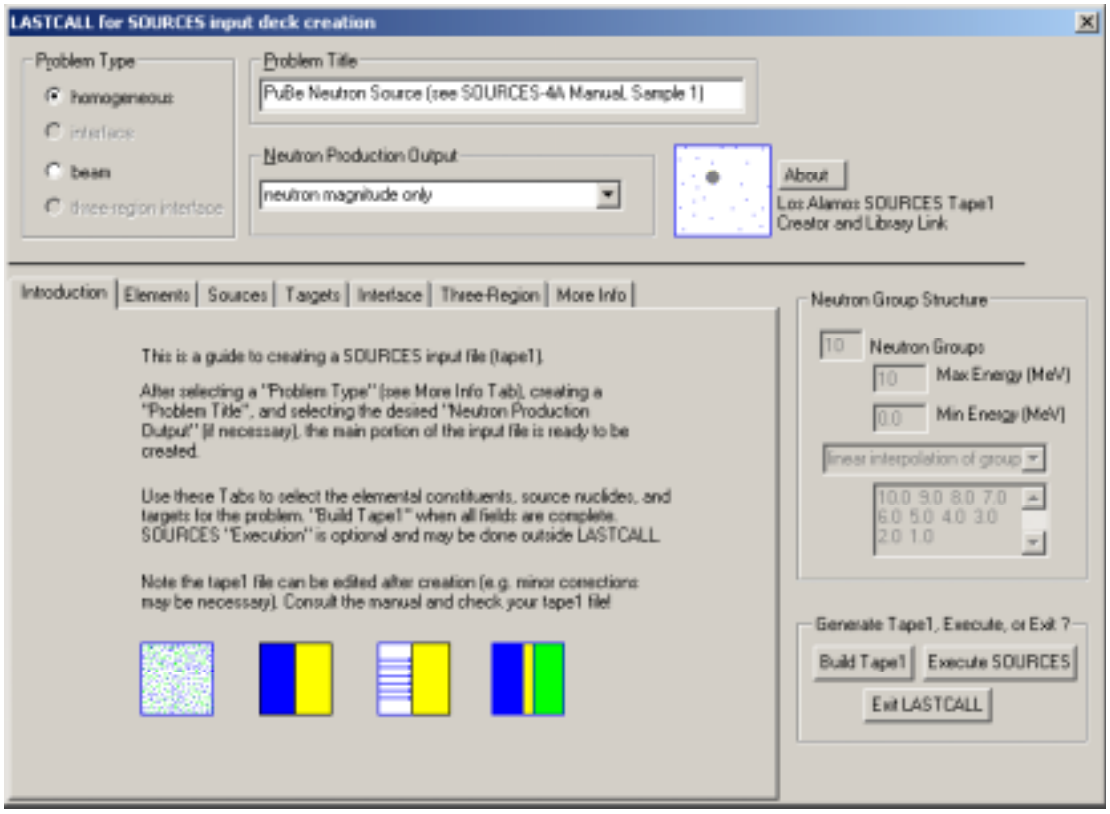

Figure 1. The default LASTCALL display upon execution.

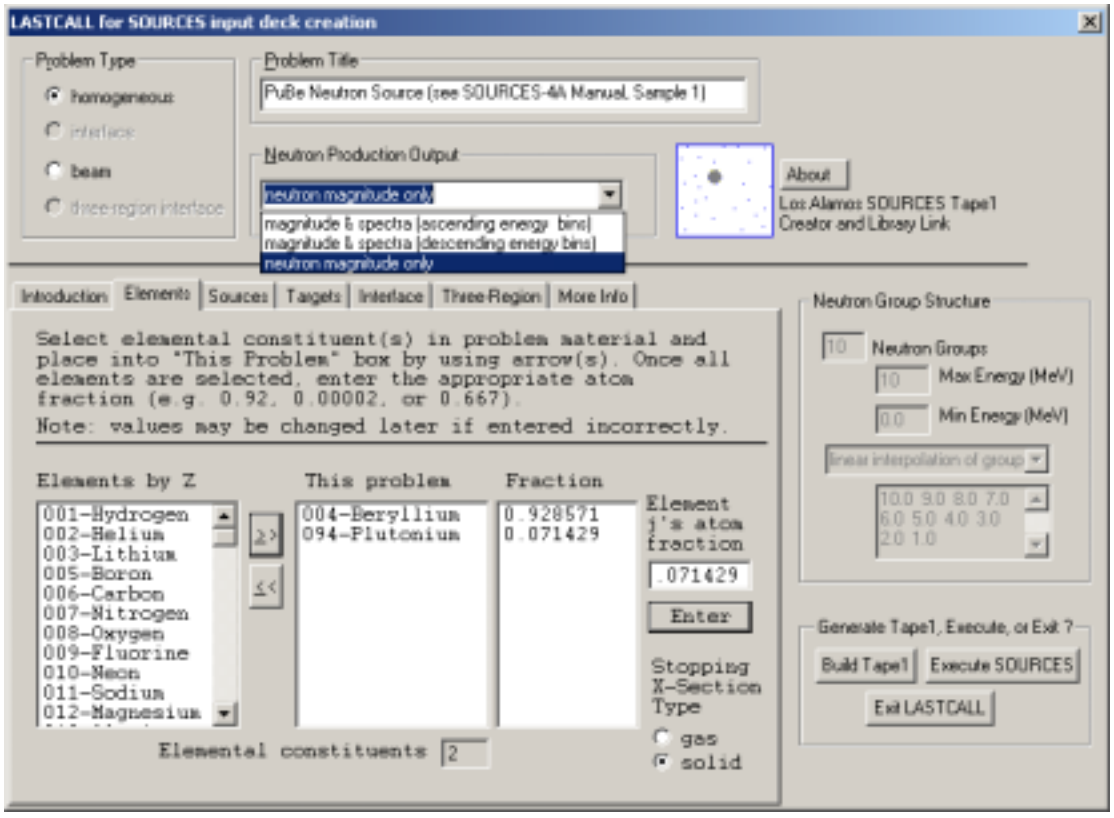

Figure 2. "Elements" tab is displayed. Note the "Neutron Production Output" selections.

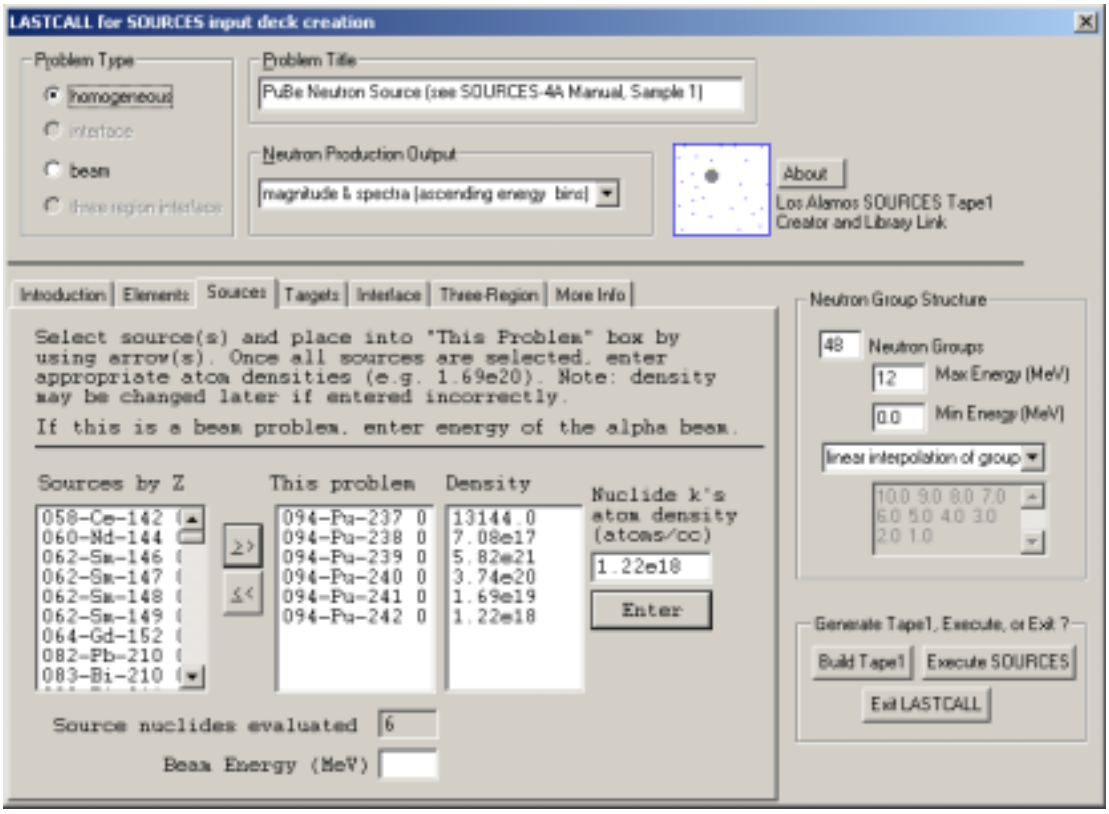

Figure 3. The "Sources" tab is displayed. Six plutonium source isotopes were chosen selected.

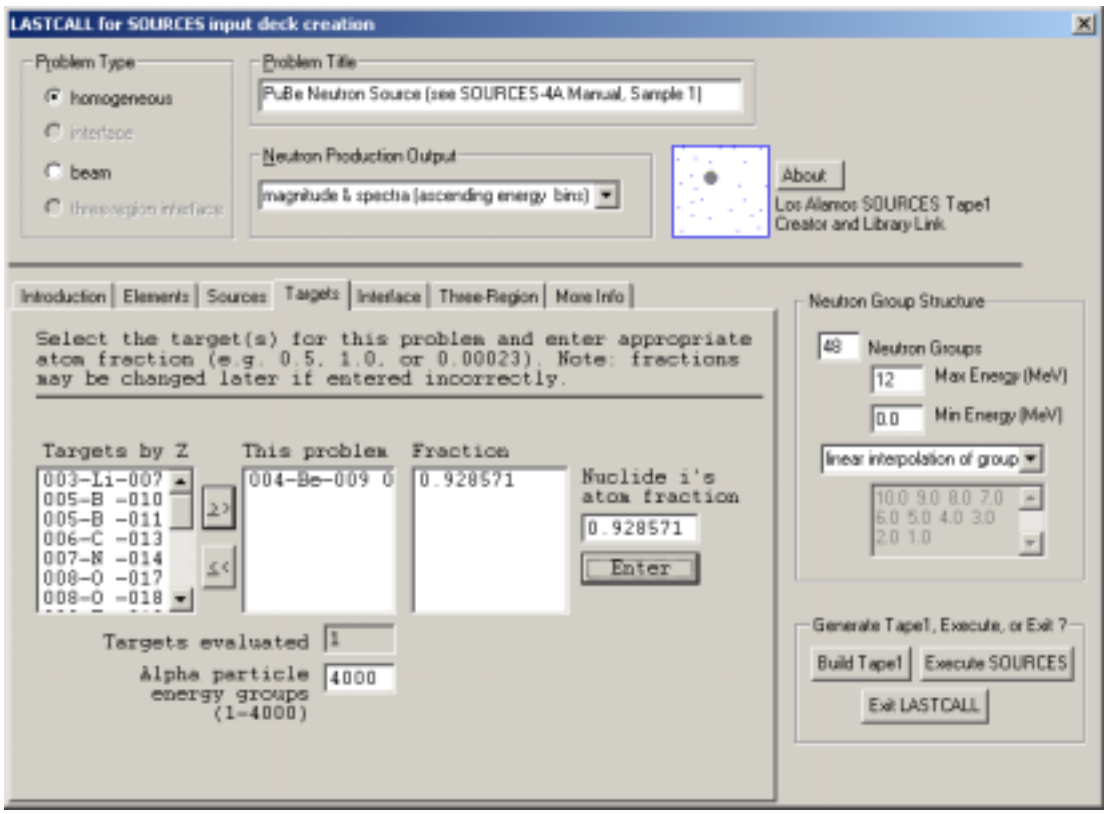

Figure 4. Beryllium was selected on the "Target" tab.

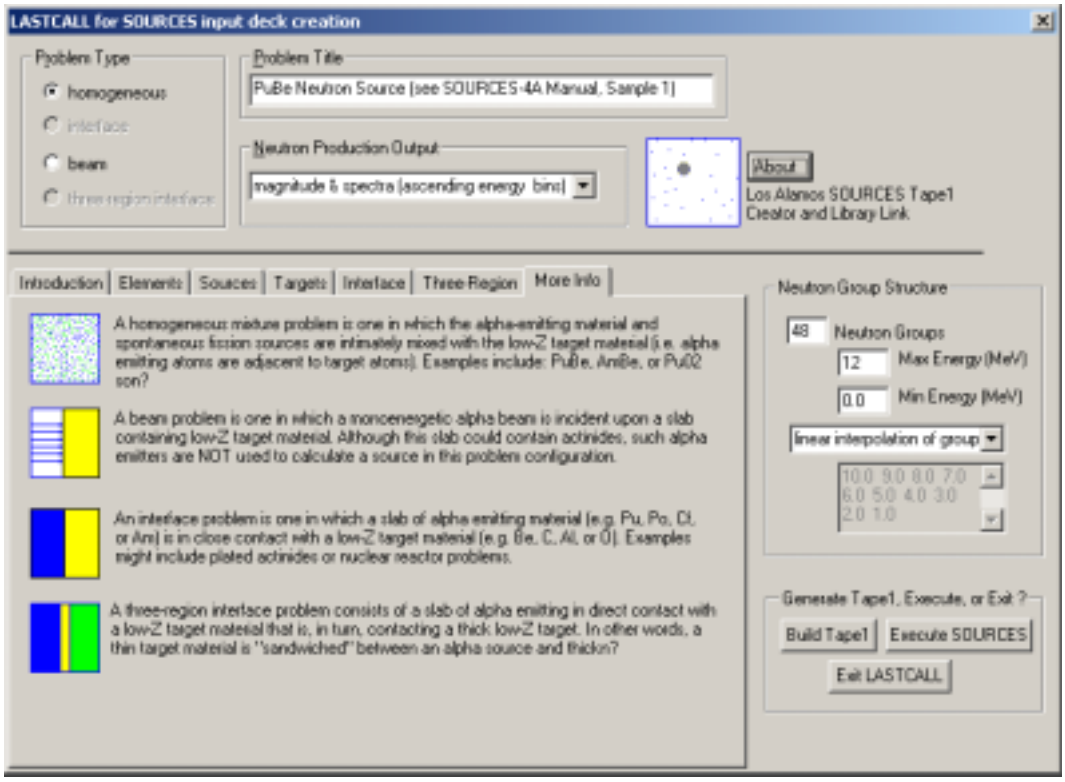

Figure 5. Additional information regarding problem types may be found on the "More Info" tab.

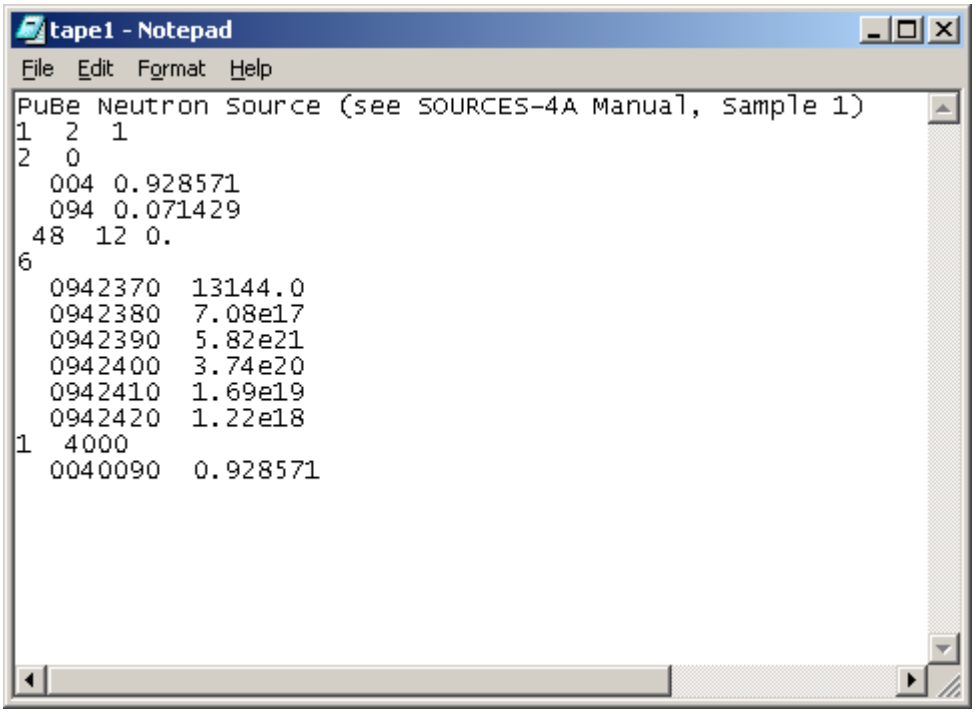

Figure 6. The product of "Building Tape1" is the automatic opening of the Notepad application to display tape1. This example is nearly identical to "Sample Problem #1" in the SOURCES manual.

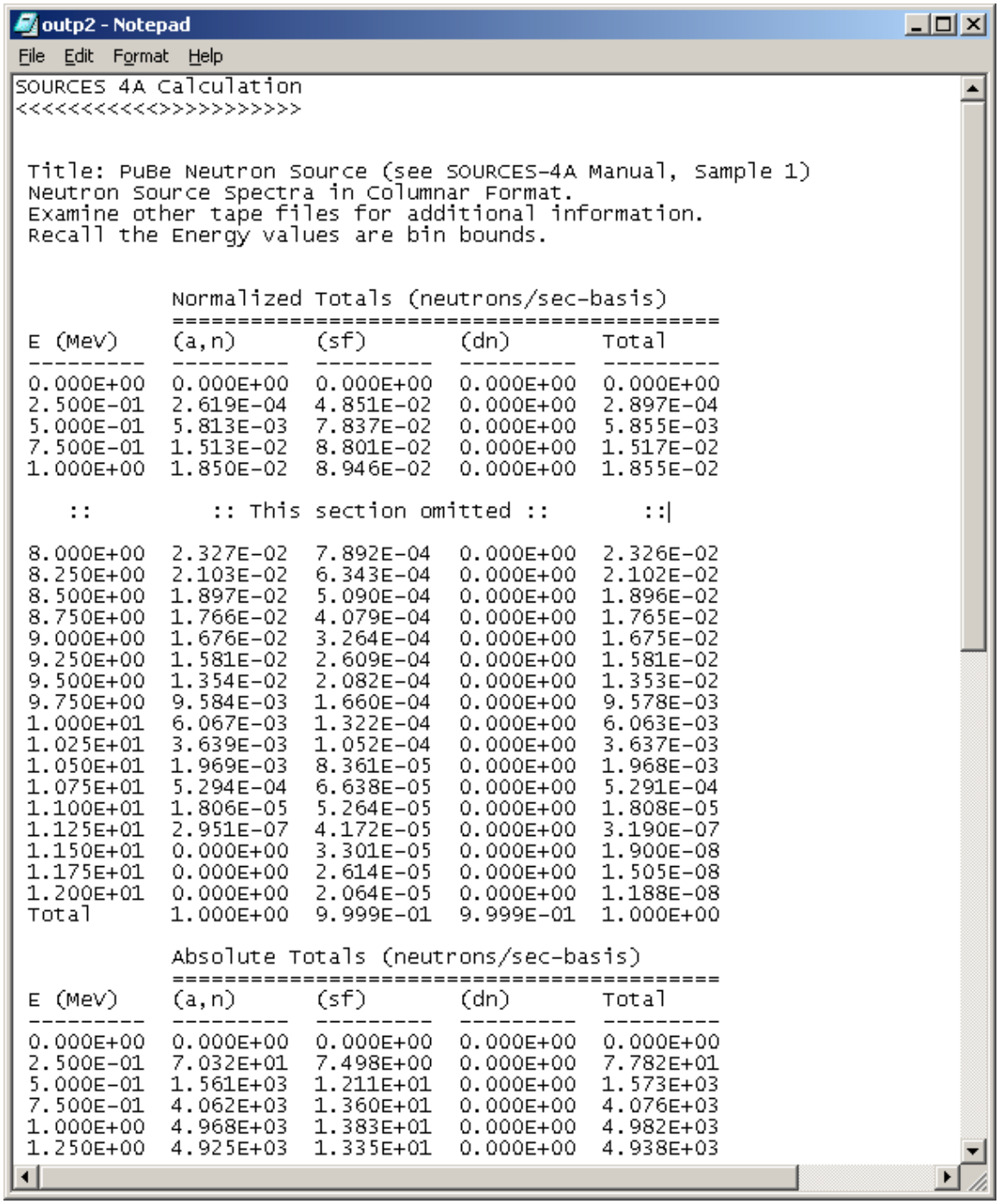

Figure 7. A new output file (outp2) displays ascending energy structure and columnar format for easier post manipulation.

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